Hierarchical Self-Assembly of a Biomimetic Light-Harvesting Antenna Based on DNA G-Quadruplexes

Oltra, Nuria Sancho; Browne, Wesley R.; Roelfes, Gerard

Published in:
Chemistry

DOI:
10.1002/chem.201202550

Publication date:
2013

CHEMISTRY
A EUROPEAN JOURNAL

Supporting Information

Hierarchical Self-Assembly of a Biomimetic Light-Harvesting Antenna Based on DNA G-Quadruplexes

Núria Sancho Oltra, Wesley R. Browne,* and Gerard Roelfes*[a]

chem_201202550_sm_miscellaneous_information.pdf

Calculation of the Förster radius.

The Förster radius was calculated in Å using the formula:

$$R_0^6 = 0.211 \cdot \left(QY_1 \cdot J(l) \cdot \frac{k^2}{n^4} \right)$$

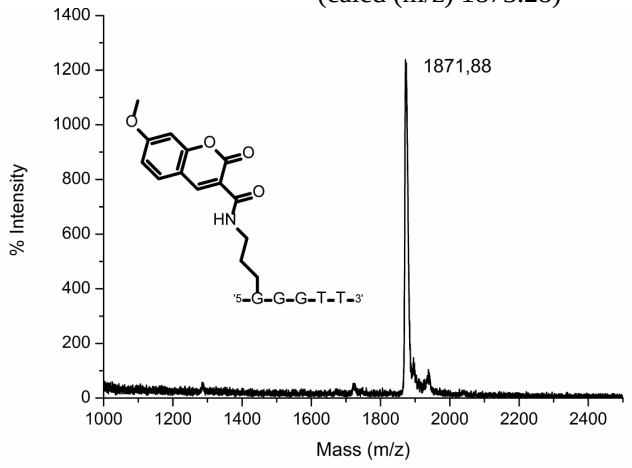
Where QY_1 is the quantum yield of fluorescence of the donor in the absence of the acceptor, n is the refractive index of the solvent and $?^2$ is the orientation between the dipoles of the chromophores. When the orientation is not known a value of 2/3 is used, which means that the relative orientation averaged over all donor-acceptor pairs is assumed to be random. $J(?)$ is the overlap integral which is calculated using the emission spectrum of the donor chromophore, normalized to unit area, and the absorption spectrum of the accepting chromophore:

$$J(l) = \int_0^\infty f_D(l) \cdot e_A(l) \cdot l^4 \, dl$$

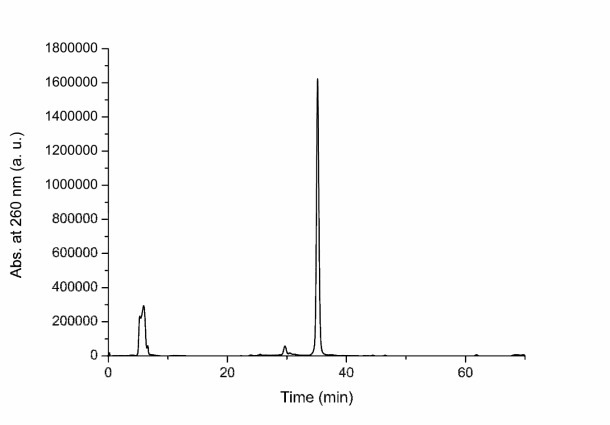
Where $f_D(l)$ is the overlap of the donor fluorescence spectrum expressed in units of $M^{-1}cm^{-1}(nm)^4$, $e_A(l)$ is the acceptor absorption spectrum expressed in units of $M^{-1}cm^{-1}$ and $?$ in nm.

Characterization of oligonucleotide conjugates.

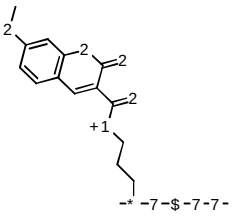
MALDI-TOF:
(calcd (m/z) 1873.28)



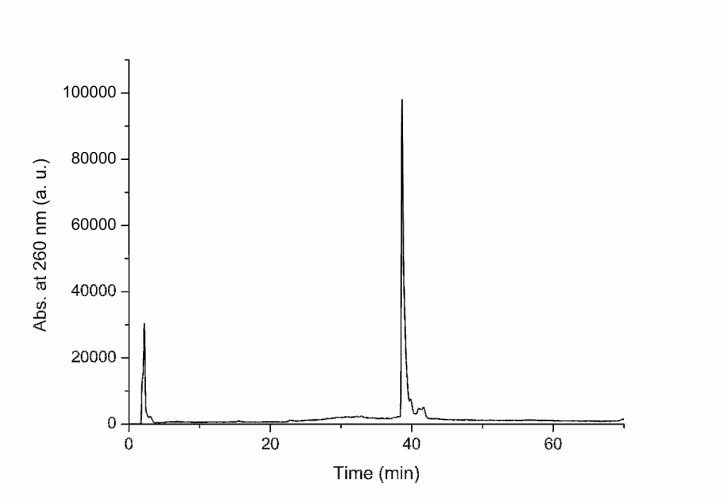
Rp-HPLC:



ESI (m/z) = 1873.4 (calcd 1873.28)



Rp-HPLC:



ESI (m/z) = 1831.60 (calcd 1832.26)

Titration G-quadruplex – H_2TMPyP4

1 mL of a solution 0.8 µM of H_2TMPyP4 in 10 mM Tris-HCl, 80 mM KCl, pH 7.3 buffer was titrated with increasing amounts of quadruplex from a 6.14 µM stock solution in the same buffer.

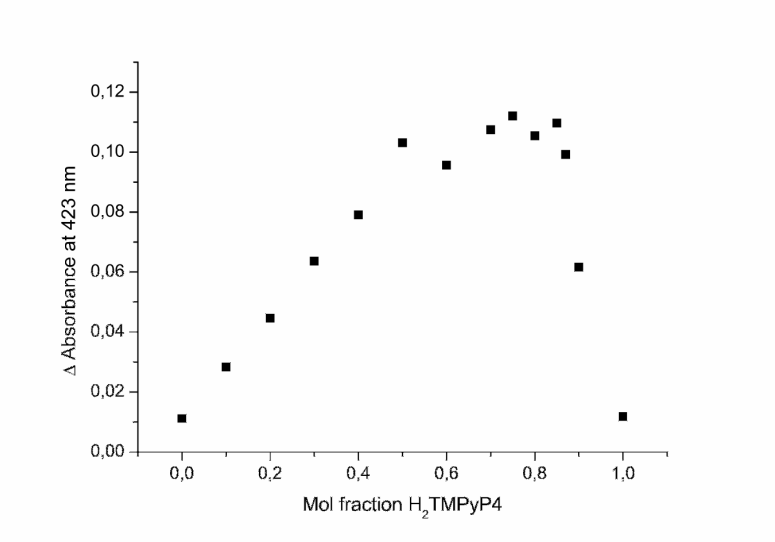


Figure S1. Job plot for the binding of **H_2TMPyP4** to *d(G_3T_2)$_4$

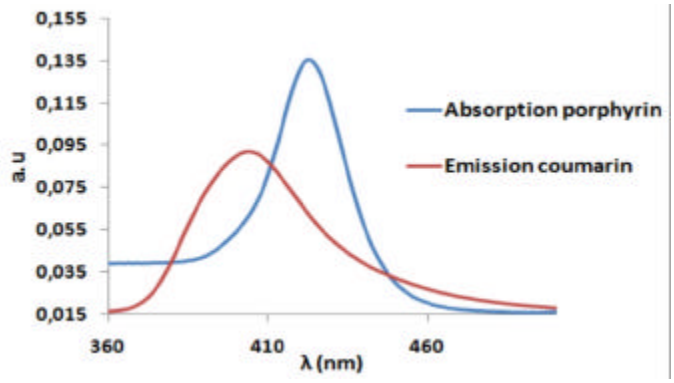


Figure S2. Overlap between the emission spectrum of the coumarin and the absorption spectrum of the porphyrin.

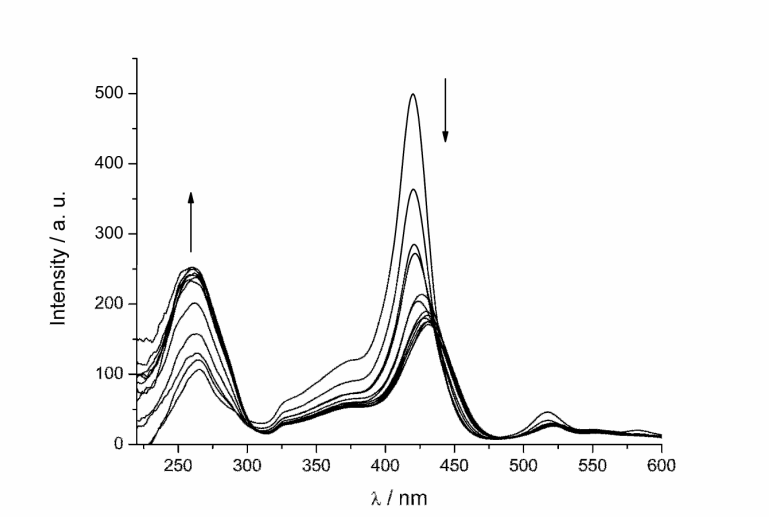


Figure S3. Excitation spectra (at ?$_{em}$ = 671 nm) of **H_2TMPyP4** in a KCl buffer in the presence of increasing amounts (0-2.3 eq.) of amino-modified quadruplex d(G_3T_2)$_4$.